

# Isophthalic acid, 4-methylpent-2-yl octyl ester

<b>Inchi:</b>	InChI=1S/C22H34O4/c1-5-6-7-8-9-10-14-25-21(23)19-12-11-13-20(16-19)22(24)26-18(4
<b>InchiKey:</b>	UPCGEBZTOLFCRT-UHFFFAOYSA-N
<b>Formula:</b>	C22H34O4
<b>SMILES:</b>	CCCCCCCCOC(=O)c1cccc(C(=O)OC(C)CC(C)C)c1
<b>Mol. weight [g/mol]:</b>	362.50

## Physical Properties

Property code	Value	Unit	Source
gf	-235.58	kJ/mol	Joback Method
hf	-772.51	kJ/mol	Joback Method
hfus	44.92	kJ/mol	Joback Method
hvap	85.04	kJ/mol	Joback Method
log10ws	-6.85		Crippen Method
logp	5.795		Crippen Method
mcvol	311.960	ml/mol	McGowan Method
pc	1184.16	kPa	Joback Method
rinpol	2501.00		NIST Webbook
tb	886.12	K	Joback Method
tc	1091.62	K	Joback Method
tf	490.96	K	Joback Method
vc	1.196	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	998.25	J/molxK	886.12	Joback Method
cpg	1069.24	J/molxK	1057.37	Joback Method
cpg	1057.48	J/molxK	1023.12	Joback Method
cpg	1044.54	J/molxK	988.87	Joback Method
cpg	1030.37	J/molxK	954.62	Joback Method
cpg	1014.95	J/molxK	920.37	Joback Method
cpg	1079.83	J/molxK	1091.62	Joback Method
dvisc	0.0000345	Paxs	886.12	Joback Method
dvisc	0.0000460	Paxs	820.26	Joback Method

dvisc	0.0000645	Paxs	754.40	Joback Method
dvisc	0.0000965	Paxs	688.54	Joback Method
dvisc	0.0001572	Paxs	622.68	Joback Method
dvisc	0.0002874	Paxs	556.82	Joback Method
dvisc	0.0006178	Paxs	490.96	Joback Method

## Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U356445&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U356445&amp;Units=SI</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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